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87018-26-6 | DTXSID30236077

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 79.4 °C

Global applicability domain: Inside

Local applicability domain index: 6.96e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

Image not found

2,3-Dimethyl-1,4-naphthoquinone
Measured: 127
Predicted: 108

Image not found

Menadione
Measured: 107
Predicted: 108